

# Electron shell and the $\alpha$ -decay

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The ratio of the  $\alpha$ -decay widths of a bare nucleus and the related atom is calculated. Both the change of the form and thus the penetrability of the potential barrier and the effect of reflection in the classically-allowed region appearing due to the electron shell are taken into account in the calculations of this ratio. The contribution of each of these two effects is of one and the same order of magnitude. For long-lived radioactive samples the values of the total effect turn out to be somewhat below 1 percent.

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## I. INTRODUCTION

Transmutation of long-lived radioactive isotopes is one of the hottest problem of the modern nuclear physics. Recent attempts to produce an affect upon the decay rate of such isotopes by physical methods which do not deal with any beam of neutrons, gamma-quanta or charged particles demonstrate increasing interest and popularity of this problem. By now a list (not so wide) of examples demonstrating the possibilities to vary the rate of  $\beta$ -transitions by deep ionization of atoms is known [1, 2]. Also it is shown that the half-life times of some low-energy  $\gamma$ -transitions turn out to be much smaller when the energy of the nuclear transition is close to the energy of any allowed atomic transition of the same multipolarity [3, 4]. The  $\alpha$ -decay looks as a process which is the most insensitive to the external influence of the discussed type due to the typical value of the energy of the potential barrier which is in the neighborhood of 20 MeV. That is why this process attracts the smaller interest than other types of decay. Nevertheless in the last decade some theoretical papers devoted to this problem were published [5, 6]. Moreover an interesting supporting evidence is obtained in the experiment presented in Ref. [7]. The difference between the decay widths of  $^{212}\text{Po}$  in Pb and Ni matrixes is proved there with 95 per cent reliability (see the discussion bellow). Thus, in our opinion, it is necessary to study accurately the effects modifying the  $\alpha$ -decay widths.

In the present paper the  $\alpha$ -decay widths of a bare nucleus and the respective atom are compared. The electron cloud changes, first, the kinetic energy of the emitted  $\alpha$ -particle and, second, the decay rate. The effect of the kinetic energy difference in cases of the decays of the bare nucleus and the atom is well-known from the middle of the last century. As usual nuclear data tables contain the values of energy yield of the  $\alpha$ -decay of atoms. Therefore the effect can not be neglected and should be accurately considered: the formal inclusion of such energy correction leads to increasing of the  $\alpha$ -decay width by the factor lying between 1.22 (for  $^{212}\text{Po}$ ) and 2.60 (for  $^{147}\text{Sm}$ ) [8]. This circumstance is always taken into account. The problem how the decay rate is changed by the electron

cloud has not solved accurately up to now.

A closely related problem is examined in Ref. [6]. To some extent paper [6] is a reaction of scientific community to mass media publications in which the  $\alpha$ -decay enhancement is anticipated in the conditions, similar to that discussed by the proponents of the so-called "cold fusion". The paper provides a qualitative argument against these anticipations. It is shown that the upper limit of the ratio of the  $\alpha$ -decay half-lives of a nucleus screened by electrons of a surrounding dense medium and the respective unscreened nucleus in actual cases is not larger than 1.02. At the same time the author does not decide between two results obtained for two versions of the screening ( $\sim 1.013$  and  $1.000$  in  $^{226}\text{Ra}$ ) i. e. between the modest and zero effects. Some other details of the investigations which is carried out in Ref. [6] are discussed bellow. So in our opinion the outlined above problem has been unresolved till now.

## II. STATEMENT OF THE PROBLEM AND FORMALISM

It is convenient to begin consideration of the problem with a simple quasi-classical approximation. The potential of the interaction of the  $\alpha$ -particle with the atomic shells is monotonically increasing negative function  $V_{sh}(r)$ , very slowly varying in the potential barrier region. Neglecting the  $r$ -dependence of the potential in this region (assuming  $V_{sh}(r) = -V_0$ ), one obtains the only effect of the shift (equal to  $V_0$ ) of the decay energy. As it is pointed out in Ref. [6] the  $\alpha$ -decay width remains the same. A small increase of the  $V_{sh}(r)$  results in increasing of the barrier height and consequently in the decreasing of the barrier penetrability which takes the form:

$$P_{at} = \exp \left[ -\frac{1}{\hbar} \int_{r_{int}}^{r_{ext}} \sqrt{V_{bn}(r) + V_{sh}(r) - E_{bn} + V_0} dr \right], \quad (1)$$

where  $E_{bn}$  is the resonance energy in the bare nucleus case,  $V_{bn}(r) = V_{str}(r) + V_{cf} + V_{Coul}(r)$  is the sum of the

strong, the centrifugal, and the Coulomb potentials of the interaction of the  $\alpha$ -particle and the residual nucleus.

At the same time there is another effect originated by the atomic shell. It appears due to the fact that the asymptotic behavior of the resonance (Gamow) wave function in the case of bare nucleus differs from that of the respective atom. Indeed, the asymptotic behavior of a resonant function looks as follows:

$$\chi_l^{res}(r) = D[G_l(\eta, kr) + iF_l(\eta, kr)], \quad r \rightarrow \infty, \quad (2)$$

where  $G_l(\eta, \rho)$  and  $F_l(\eta, \rho)$  are the Coulomb wave functions [11],

$$\eta = (e_0^2/\hbar c)Z_1Z_2\sqrt{\mu c^2/(2E)} \quad (3)$$

is the Coulomb parameter,  $e_0 > 0$  – the elementary charge,  $E$  – the decay energy yield,  $k$  – the respective wave number, and  $\mu$  – the reduced mass,  $Z_2 = 2$  – the  $\alpha$ -particle charge. The coefficient

$$D = \sqrt{\mu\Gamma}/\hbar, \quad (4)$$

determines the decay width  $\Gamma$ . In the case of bare nucleus the parameters  $D_{bn}$ ,  $\eta_{bn}$ , and  $k_{bn}$  are related to the energy  $E_{bn}$  and the charge of the daughter nucleus  $Z_1 = Z-2$  whereas the corresponding parameters  $\eta_{at}$  and  $k_{at}$  (the case of neutral atom) are related to the energy  $E_{at} = E_{bn} - V_0$  and the charge  $Z_1 = -2$  of the residual system – the nucleus and the electron cloud. The origin of the discussed effect is the reflection of the  $\alpha$ -particle wave on the varying potential. An obvious way to account for this effect is to solve the Schrödinger equation directly. It may be found grater or smaller than the effect of the barrier form variation considered above. The main goal of the present paper is to calculate the ratio of the decay width, accounting for both these effects.

A physical model applied here for the description of the  $\alpha$ -decay of the atomic system includes the following ingredients.

First, the distribution of the electronic cloud is assumed to be undistorted during the  $\alpha$ -particle emission. This assumption is based on the facts that the orbits of the strongly bound electrons are slightly changed due to the variation of the nuclear charge  $Z \rightarrow Z - 2$  and the weakly bound electrons are too slow. Indeed, the electron velocity  $v_e \approx v_\alpha$  ( $v_\alpha$  is a velocity typical for the  $\alpha$ -particle) corresponds to the electron energy  $E_e \approx 500$  eV. Thus a high speed and a small charge of the emitted particle enables one to represent the potential energy term of the Hamiltonian in the folding-form interaction of the  $\alpha$ -particle with negative ion consisting of the daughter nucleus and the atomic shell of the mother one.

Second, the electron distribution is taken in the Thomas-Fermi form [9].

Third, the electron charge, associated with sphere of the radius  $R_0$  which is somewhat greater than that of the range of strong interaction  $R_{str} \sim [1.2A^{1/3} + R_\alpha + 2]$  fm, is assumed to be small enough to neglect the variation of the potential originated by this charge.

At last only the ratio of the  $\alpha$ -decay widths but not the absolute values of the widths for both an atom and a bare nucleus is the object of the calculation. Evidently the absolute values are related to many-nucleon properties of a nucleus and thus are beyond the scope of the present paper.

The properties of the Gamov solutions to the two-body Schrödinger equation related to the presented model are the following. The solution is characterized by the asymptotic form (2) with the parameters  $D_{at}$ ,  $\eta_{at}$ , and  $k_{at}$  at very large (several times grater than the atomic radius) distances. At smaller distances it can be obtained only numerically. In the region  $R_{str} < r < R_0$  the equation turns out to be the Coulomb one with the parameters  $\eta_{bn}$  and  $k_{bn}$  related to the bare nucleus. Consequently in this domain the resonance solution becomes:

$$\chi_l^{res}(r) = D_{at}[AG_l(\eta_{bn}, k_{bn}r) + BF_l(\eta_{bn}, k_{bn}r)]. \quad (5)$$

In this region the coefficients  $D_{at}$ ,  $A$ , and  $B$  differ the solution from the one, corresponds to the Gamow state of bare nucleus, where  $D = D_{bn}$ ,  $A = 1$ , and  $B = i$  (see Eq. (2)).

In the both cases the amplitude of each wave function is determined by the matching of the function of the type (5) with one and the same internal wave function. As it is shown in the Ref. [10] the term containing the regular Coulomb function plays a negligible role in the decay width calculations of a narrow resonance. Indeed, the ratio of the regular and the irregular Coulomb wave functions in the sub-barrier region can be estimated as follows:

$$F_l(\eta_{bn}, k_{bn}r)/G_l(\eta_{bn}, k_{bn}r) \cong P(r) = \exp \left[ -\frac{1}{\hbar} \int_r^{r_{ext}} \sqrt{E - V(\rho)} d\rho \right], \quad r \ll r_{ext}. \quad (6)$$

Remind that for the  $\alpha$ -emitters with the half-lives  $\tau > 1$  y the value of the total penetrability of the barrier (which is expressed by Eq. (6) with the lower limit  $r = r_{int}$ )  $P < 10^{-27}$ . Furthermore, the region beyond the radius  $R_{str}$  contributes predominantly to the value of the integral in Eq. (6). Thus, the second term in Eq. (5) can be neglected with a high precision. Therefore the squared ratio of the amplitudes of the wave functions and consequently the ratio of the widths become

$$\Gamma_{bn}/\Gamma_{at} = |D_{bn}/D_{at}|^2 = |A|^2 \quad (7)$$

This coefficient should be calculated numerically. The calculation procedure is complicated due to the need to solve numerically Schrödinger equation in extremely wide domain of values of the radial variable  $r$ . The results of the performed calculations demonstrate that the asymptotic form (2) becomes valid at the distance of the order of  $10^6$  fm whereas a typical value of the wave number of the  $\alpha$ -particle is about  $k \simeq 1$  fm $^{-1}$ . At the same time a

high numerical precision should be provided both at the large distance and in the neighborhood of the nucleus. In fact one deals with two very different scales of distances in one and the same calculation procedure.

The optimal way is as follows. As it is noted above one has no need to solve the Schrödinger equation in the  $r \leq R_{str}$  region for the calculation of the ratio of the decay widths of an atom and the respective bare nucleus – this ratio is determined beyond the region. Therefore it is convenient to consider the reduced equation:

$$\left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_{Coul}(r) + V_{sh}(r) + V_{cf}(r) - E \right) \chi_l(r) = 0. \quad (8)$$

The Thomas-Fermi model was utilized for description of the electron cloud potential:

$$V_{sh}(r) = 2\varphi_{sh}(r)e_0, \quad (9)$$

$$\varphi_{sh}(r) = \frac{-Ze_0}{r}(1 - \xi(x)), \quad (10)$$

$x = rZ^{1/2}m_e e_0^2 b^{-1} \hbar^{-2}$ ,  $b = (3\pi/4)^{2/3}/2$  ( $m_e$  – electron mass). In this case  $V_0 = 2m_e Z^{4/3} e_0^4 \kappa b^{-1} \hbar^{-2}$  and  $\kappa \approx 1.59$  is the constant in the asymptotic formula  $\xi(x) \simeq 1 - \kappa x$ , as  $x \rightarrow 0$ . We introduce the distance  $R_0$  in such a way that in the domain  $r < R_0$  the  $r$ -dependence of  $V_{sh}$  can be neglected:  $V_{sh}(r) \cong -V_0$ . Thus in the domain  $R_{str} < r < R_0$  equation (8) takes the form

$$\frac{d^2 \chi_l(r)}{dr^2} + \left( \frac{2\mu E_{bn}}{\hbar^2} - \frac{4\mu(Z-2)e_0^2}{\hbar^2 r} - \frac{l(l+1)}{r^2} \right) \chi_l(r) = 0. \quad (11)$$

This equation coincides with that in the case of bare nucleus but with shifted energy  $E_{bn}$ .

The Coulomb wave functions  $F_l(\eta_{bn}, k_{bn}r)$  and  $G_l(\eta_{bn}, k_{bn}r)$  are the solutions to Eq. (11). Thus the two linearly independent solutions to Eq. (8) can be chosen in the following way

$$\chi_l^{(F)}(r) = F_l(\eta_{bn}, k_{bn}r), \quad R_{str} < r < R_0, \quad (12)$$

$$\chi_l^{(G)}(r) = G_l(\eta_{bn}, k_{bn}r), \quad R_{str} < r < R_0. \quad (13)$$

At large distances, far from the electron shells the sum of potentials of electron shells and nucleus looks like the potential of negative ion with the charge  $Z_1 = -2$ . In this region the solutions to Eq. (8) have the form of linear combinations of functions  $F_l(\eta_{at}, k_{at}r)$  and  $G_l(\eta_{at}, k_{at}r)$ :

$$\chi_l^{(F)}(r) = \alpha F_l(\eta_{at}, k_{at}r) + \beta G_l(\eta_{at}, k_{at}r), \quad (14)$$

$$\chi_l^{(G)}(r) = \gamma F_l(\eta_{at}, k_{at}r) + \delta G_l(\eta_{at}, k_{at}r). \quad (15)$$

The reversed relationships

$$F_l(\eta_{at}, k_{at}r) = [\delta \chi_l^{(F)}(r) - \beta \chi_l^{(G)}(r)]/\Delta, \quad (16)$$

$$G_l(\eta_{at}, k_{at}r) = [-\gamma \chi_l^{(F)}(r) + \alpha \chi_l^{(G)}(r)]/\Delta, \quad (17)$$

$$\Delta = \alpha\delta - \beta\gamma \quad (18)$$

follow directly from Eqs. (14) and (15). The value of  $\Delta$  can be found without explicit values of  $\alpha, \beta, \delta, \gamma$ . Indeed, the relationship

$$W_r(\chi_l^{(F)}, \chi_l^{(G)}) = W_r(F_l(\eta_{at}, k_{at}r), G_l(\eta_{at}, k_{at}r))\Delta \quad (19)$$

follows directly from (14), (15), and (18). The lower index  $r$  means that the derivatives with respect to variable  $r$  appear in the Wronskian  $W_r$ . As it is known [11]

$$W_\rho(F_l(\eta, \rho), G_l(\eta, \rho)) = 1, \quad (20)$$

so from (12), (13), and (19) it follows that

$$\Delta = k_{bn}/k_{at}. \quad (21)$$

In the case of  $\alpha$ -decay of a neutral atom the resonant wave function has the asymptotic form  $D_{at}[G_l(\eta_{at}, k_{at}r) + iF_l(\eta_{at}, k_{at}r)]$  at large distances far from the electron shells. Now, with the aid of (16), (17) it is clear that the considered resonance wave function looks as follows

$$\chi_l^{res} = D_{at} \left[ \frac{\alpha - i\beta}{\Delta} \chi_l^{(G)} + i \frac{\delta + i\gamma}{\Delta} \chi_l^{(F)} \right]. \quad (22)$$

The function (22) in the domain  $R_{str} < r < R_0$  has the form (see (12), (13)):

$$D_{at} \left[ \frac{\alpha - i\beta}{\Delta} G_l(\eta_{bn}, k_{bn}r) + i \frac{\delta + i\gamma}{\Delta} F_l(\eta_{bn}, k_{bn}r) \right]. \quad (23)$$

Thus, we come to the following conclusion. In the case of the neutral atom the internal wave function must be matched with the function (23), while in the case of the bare nucleus with the function  $D_{at}[G_l(\eta_{bn}, k_{bn}r) + iF_l(\eta_{bn}, k_{bn}r)]$ . The matching procedure can be realized at any point of the domain  $R_{str} < r < R_0$ .

In the case of neutral atom the multiplier of  $G_l(\eta_{bn}, k_{bn}r)$  in Eq. (23), which is symbolized as  $A$  in Eqs. (5) and (7), changes the width of the resonant state. Obviously there is no need to solve the resonant problem as a whole to determine the coefficient  $A$ . It is sufficient to solve (numerically) the Schrödinger equation (8) in the domain  $r > R_{str}$  with the boundary condition (12). Then the coefficients  $\alpha$  and  $\beta$  can be deduced from the Wronskians of the solution and the functions  $G_l(\eta_{at}, k_{at}r)$  and  $F_l(\eta_{at}, k_{at}r)$ . The explicit expression

$$\Gamma_{bn}/\Gamma_{at} = |(\alpha - i\beta)/\Delta|^2 = (\alpha^2 + \beta^2)/\Delta^2 \quad (24)$$

for the suppression factor – the ratio of the decay width of the bare nucleus and the neutral atom – follows directly from (4) and (5). It should be pointed out that we arrived at a surprising conclusion. Indeed, one needs to find the solution with boundary condition (12) (regular function  $F_l(\eta_{at}, k_{at}r)$ ) to calculate the coefficient in the term containing the irregular function  $G_l(\eta_{at}, k_{at}r)$ .

### III. RESULTS AND DISCUSSION

The influence of the electron surrounding onto the  $\alpha$ -decay width was investigated for some isotopes in the framework of the rigorous approach described above. The Runge-Kutta and Stoermer methods were applied

Table I: The values of the coefficient of suppression of the  $\alpha$ -decay widths by the electron shell.

Isotope	$Q_{at}$	$\Gamma_{bn}/\Gamma_{at}$	$P_{bn}/P_{at}$
$^{226}\text{Ra}$	4.7806	1.0021	1.006
$^{232}\text{Th}$	4.0288	1.0052	1.010
$^{144}\text{Nd}$	1.9251	1.0079	1.014
$^{148}\text{Sm}$	1.9858	1.0085	1.015

to solve numerically the radial Schrödinger equation (8). The results obtained by means of these methods coincide with high accuracy. The factors of the  $\alpha$ -decay suppression caused by the electron shells are presented in Table I. The third column of the table demonstrates the results of precise calculations and the last one the results of quasiclassical calculations of the barrier penetrabilities. The results of exact calculations, based on Eq. (24) differ from that of quasiclassical approach. The reason of this discrepancy is the following. The ratio  $P_{bn}/P_{at}$  is the exponential function of difference of two integrals (see (1)) over the subbarrier regions. It turns out that the vicinity of the corresponding external turning points (upper limits of the integrals) contributes predominantly to the difference of the quasiclassical integrals. But the vicinity of a turning point is just the region, where the quasiclassical approximation loses accuracy.

In a qualitative sense the results presented in the table are not in contradiction with the experimental one

[7] where the following difference between the half-life times of  $^{212}\text{Po}$  decay in Pb and Ni matrixes is obtained:  $T_{1/2}(\text{Pb}) - T_{1/2}(\text{Ni}) = (-0.66 \pm 0.25)$  ns. This difference, related to the half-life time of  $^{212}\text{Po}$  isotope  $T_{1/2} = 0.3$   $\mu\text{s}$  is about 0.2 per cent. It should be stressed that the settings of the problems in the present work and in Ref. [7] are different. The effect of the change of solid state surrounding of the emitter but not the effect of the ionization is studied in the experiment. So, a direct comparison is impossible.

As it is noted above the upper limit of an  $\alpha$ -decay half-life time variation in a dense (solid or liquid) medium is estimated theoretically in Ref. [6]. The effect is assumed to be originated by the change of the quasiclassical penetrability of the barrier by the potential of the interaction of the  $\alpha$ -particle with electrons of the medium. The initial barrier is chosen in the simple form of "cut Coulomb potential". The change of the barrier is described by the exponential screening factor  $\exp(-r/R)$ . Two parameters  $R = 3.7 \cdot 10^3$  fm (for so-called "Thomas-Fermi screening") and  $R = 4 \cdot 10^5$  fm (for "Debye screening") are considered. The values  $P_{bn}/P_{at} = 1.013$  and 1.000 for  $^{226}\text{Ra}$  are obtained in these cases respectively. The larger value of the upper limit is qualitatively confirmed in our calculations.

So the ratio of the  $\alpha$ -decay widths of a bare nucleus and the related atom is calculated in accurate way. The mathematics providing a possibility to take into account the effect of reflection of the  $\alpha$ -particle wave at the electron shell in the classically-allowed region is built. The change of the penetrability of the potential barrier is taken into account simultaneously. For long-lived radioactive samples the values of the effect turn out to be somewhat below 1 percent. They decrease with increasing of the decay energy.

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